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Bounds for the Solution of the Poisson–Boltzmann Equation about a Cylindrical Particle

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Pointwise upper and lower bounds for the solution of a Dirichlet problem involving the Poisson–Boltzmann equation in cylindrical coordinates are derived from the theory of maximum principles in differential equations. Simple analytical bounding curves are obtained for various illustrative examples.

1. INTRODUCTION

The nonlinear boundary value problem

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right)=\sinh u, \qquad r>r_0>0, \tag{1.1}$$

with

$$u(r_0)=u_0>0, \qquad u\to 0 \quad \text{as} \quad r\to\infty, \tag{1.2}$$

arises in studies of the electrostatic potential u about a single, infinitely long, circular–cylindrical charged particle of radius r_0 immersed in an electrolytic solution [5]. Apart from its own intrinsic value, solutions of this problem are of considerable interest in biophysics, for example, in work on filaments in striated muscle [4]. However, exact solutions are not available of (1.1) and (1.2), and recourse must be had in some kind of approximation, using numerical or variational approaches for instance. The main drawback of approaches like these is that extensive computation is often required, and so alternative methods are desirable. One alternative, adopted by Philip and Wooding [5], involves approximating the sinh u in (1.1) by another function in such a way that the resulting problem can be solved in terms of elementary functions. Thus they take

$$\sinh u \sim u \qquad \text{if} \quad 0<u<1, \tag{1.3}$$

$$\sim \tfrac{1}{2}e^{u} \qquad \text{if} \quad u>1, \tag{1.4}$$

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and replace (1.1) and (1.2) by

(i) $0 < u_0 < 1$,

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) = u, \qquad 0 < r_0 \leqslant r < \infty, \tag{1.5}$$

$$u(r_0) = u_0, \qquad u \to 0 \quad \text{as} \quad r \to \infty, \tag{1.6}$$

(ii) $u_0 > 1$,

$$\begin{aligned} \frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right) &= \frac{1}{2}e^u, \qquad 0 < r_0 \leqslant r < r^* \\ &= u, \\ & r^* \leqslant r < \infty \end{aligned} \tag{1.7}$$

$$u(r^*) = 1, \tag{1.8}$$

$$u(r_0) = u_0, \qquad u \to 0 \quad \text{as} \quad r \to \infty, \tag{1.9}$$

$$u, du/dr \quad \text{continuous at} \quad r = r^*. \tag{1.10}$$

Case (i) corresponds to what is known as the Debye–Hückel approximation. Case (ii) leads to an elaborate scheme and has the unsatisfactory feature that at $r = r^*$ the differential equation (1.7) has a jump discontinuity in the right-hand side.

In this paper we describe another alternative in which simple analytical pointwise *bounds* on the exact solution are obtained by using the maximum principle for differential equations [6]. In this approach there are no discontinuities and the cases (i) $0 < u_0 < 1$, (ii) $u_0 > 1$ do not require separate treatment. Illustrative results are obtained for some simple cases.

2. General Pointwise Bounds

The boundary value problem can be written as

$$Lu = f(u), \qquad r > r_0 > 0, \tag{2.1}$$

$$u(r_0) = u_0 > 0, \qquad u \to 0 \quad \text{as} \quad r \to \infty. \tag{2.2}$$

where

$$Lv = \frac{1}{r}\frac{d}{dr}\left(r\frac{dv}{dr}\right), \qquad f(v) = -\sinh v. \tag{2.3}$$

At the end of this section we establish the existence and uniqueness of a solution of (2.1) and (2.2). We shall denote the solution by u.

Now suppose that two functions u_1 and u_2 can be found so that

$$\begin{aligned} &Lu_1 \leqslant f(u_1), && r > r_0 > 0, \\ &u_1(r_0) = u_0, && u_1 \to 0 \quad \text{as} \quad r \to \infty \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} &Lu_2 \geqslant f(u_2), && r > r_0 > 0 \\ &u_2(r_0) = u_0, && u_2 \to 0 \quad \text{as} \quad r \to \infty. \end{aligned} \tag{2.5}$$

Then (2.4) and (2.1) with (2.2) imply

$$\begin{aligned} L(u_1 - u) &\leqslant f(u_1) - f(u) \\ &\leqslant -K(u_1 - u) \end{aligned}$$

for $K \geqslant 0$, since $\partial f/\partial u = -\cosh u < 0$. Hence

$$(L + K)(u_1 - u) \leqslant 0,$$

implying, by the maximum principle [6], that

$$u_1 - u \leqslant 0$$

or

$$u_1 \leqslant u.$$

In the same way, with (2.5) instead of (2.4), we find that

$$u \leqslant u_2.$$

Combining these we therefore have established the upper and lower bounds

$$u_1(r) \leqslant u(r) \leqslant u_2(r), \qquad r > r_0 > 0, \tag{2.6}$$

on the exact solution $u(r)$.

One way to obtain bounding functions u_1 and u_2 in practice is to choose two functions f_1 and f_2 such that

$$f_1(u) \leqslant f(u) \qquad \text{all} \quad u, \tag{2.7}$$

and

$$f_2(u) \geqslant f(u) \qquad \text{all} \quad u, \tag{2.8}$$

and let u_1 and u_2 be solutions of

$$Lu_1 = f_1(u_1), \qquad r > r_0 > 0, \tag{2.9}$$

and

$$Lu_2 = f_2(u_2), \qquad r > r_0 > 0, \tag{2.10}$$

subject to the boundary conditions (2.2). Because of (2.7) and (2.8) the inequalities in (2.4) and (2.5) are then satisfied. The functions f_1 and f_2 can be taken to be linear functions, and so (2.9) and (2.10) are readily solved analytically for the bounding functions u_1 and u_2. This procedure for obtaining u_1 and u_2 has been exploited recently in one-dimensional problems by Villadsen and Michelson [8], by Varma and Strieder [7], and by Arthurs and co-workers [2, 3].

The existence of a solution to the problem in (2.1) and (2.2) can be established by using a result due to Amman [1]. This result concerns boundary value problems of the form

$$Lu = g(u) \qquad \text{in} \quad V, \tag{2.11}$$

$$u = \phi(u) \qquad \text{on} \quad \partial V, \tag{2.12}$$

where L denotes a positive linear operator, with

$$g(0) \geqslant 0, \qquad \phi(0) \geqslant 0. \tag{2.13}$$

In our case

$$g(u) = -\sinh u, \tag{2.14}$$

$$\begin{aligned} \phi(u) &= u_0 \qquad \text{at} \quad r = r_0 \\ &\to 0 \qquad \text{at} \quad r \to \infty \end{aligned} \tag{2.15}$$

so that conditions (2.13) are satisfied. Consequently Amman's Theorem A enables us to state that a necessary and sufficient condition for the existence of a nonnegative solution u of the boundary value problem (2.1) and (2.2) is the existence of a nonnegative C^2 function w satisfying

$$Lw \geqslant g(w), \qquad r \geqslant r_0 > 0 \tag{2.16}$$

$$w \geqslant 0 \qquad \text{on} \quad \partial[r_0, \infty). \tag{2.17}$$

To construct such a function w we consider the problem

$$Lw = g_2(w) = -w, \qquad r \geqslant r_0 > 0, \tag{2.18}$$

with

$$w(r_0) = u_0, \qquad w \to 0 \quad \text{as} \quad r \to \infty. \tag{2.19}$$

This problem has solution

$$w(r) = u_0 \frac{K_0(r)}{K_0(r_0)}, \qquad r \geqslant r_0 > 0, \tag{2.20}$$

where K_0 is a modified Bessel function of the second kind (cf. [9]). The function in (2.20) is nonnegative and for such a function

$$g_2(w) \geqslant g(w) \tag{2.21}$$

so that (2.16) is satisfied. Further, (2.19) implies (2.17), and hence the function in (2.20) satisfies (2.16) and (2.17). By Amman's theorem we have therefore established the existence of a nonnegative solution of the problem in (2.1) and (2.2).

To show that the solution u of (2.1) and (2.2) is unique we suppose the contrary and let u_α and u_β denote two distinct solutions of the boundary value problem. If we define the quantity

$$P_{\alpha\beta} = \int_{r_0}^{\infty} \left[\left\{ \frac{d}{dr}(u_\alpha - u_\beta) \right\}^2 + (u_\alpha - u_\beta)(\sinh u_\alpha - \sinh u_\beta) \right] r dr, \tag{2.22}$$

we see that for any distinct functions u_α and u_β

$$P_{\alpha\beta} > 0. \tag{2.23}$$

But, integrating the d/dr term in (2.22) by parts, we have

$$P_{\alpha\beta} = \int_{r_0}^{\infty} (u_\alpha - u_\beta)\{L(u_\alpha - u_\beta) + \sinh u_\alpha - \sinh u_\beta\} r dr + \left[(u_\alpha - u_\beta) r \frac{d}{dr}(u_\alpha - u_\beta) \right]_{r_0}^{\infty} \tag{2.24}$$

and if u_α and u_β are distinct solutions of (2.1) and (2.2) then

$$P_{\alpha\beta} = 0, \tag{2.25}$$

which contradicts (2.23). Hence the solution of (2.1) and (2.2) is unique.

3. Pointwise Bounds 1

To guide us in our initial choice of suitable functions f_1 and f_2 for use in (2.9) and (2.10), we show in Fig. 1 the appropriate part of the function

$$f(u) = -\sinh u \tag{3.1}$$

corresponding to the region

$$0 \leqslant u \leqslant u_0. \tag{3.2}$$

3.1. *Lower Bounding Function*

To obtain a pointwise lower bound u_1 for u we choose the function $f_1(u)$ as the chord joining the points $(0, 0)$ and $(u_0, -\sinh u_0)$ in the $u, f(u)$ plane. This line lies below the function $f(u) = -\sinh u$ in the region specified by (3.2) and is given by

$$f_1(u) = -k^2 u, \tag{3.3}$$

with

$$k^2 = \frac{\sinh u_0}{u_0}. \tag{3.4}$$

For this choice of $f_1(u)$ the inequality (2.7) holds and by (2.9) the function u_1 satisfies

$$Lu_1 = -k^2 u_1, \qquad r \geqslant r_0 > 0, \tag{3.5}$$

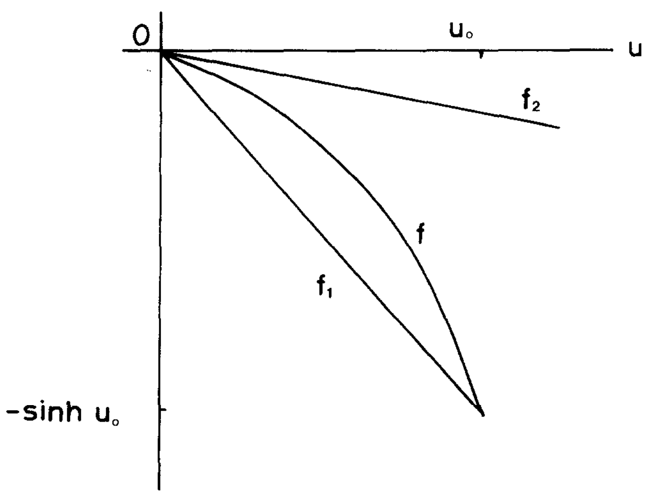

Fig. 1. Functions f, f_1 and f_2.

subject to

$$u_1(r_0) = u_0, \qquad u_1 \to 0 \quad \text{as} \quad r \to \infty. \tag{3.6}$$

Equations (3.5) and (3.6) have the solution

$$u_1(r) = u_0 \frac{K_0(kr)}{K_0(kr_0)} = u_1^{(1)}(r) \qquad \text{say,} \tag{3.7}$$

which from the theory of Section 2 is a lower bounding function for the exact solution u of (1.1) and (1.2). Here K_0 is a modified Bessel function of the second kind given by (cf. [9, p. 374])

$$K_0(z) = -\sum_{r=0}^{\infty} \frac{(\frac{1}{2}z)^{2r}}{(r!)^2} \left\{ \log \frac{1}{2} z + \gamma - \sum_{m=1}^{r} m^{-1} \right\} \tag{3.8}$$

as an ascending series.

3.2. *Upper Bounding Function*

To obtain a pointwise upper bound u_2 for u we choose the function $f_2(u)$ as the tangent to $f(u)$ at the point $(0, f(0))$. From Fig. 1 we see that this tangent lies above $f(u)$ for nonnegative u and is given by

$$f_2(u) = -k_2^2 u, \tag{3.9}$$

where

$$k_2^2 = -f'(0) = 1. \tag{3.10}$$

For this choice of $f_2(u)$ the inequality (2.8) holds and by (2.10) the function u_2 satisfies

$$Lu_2 = -u_2, \qquad r \geqslant r_0 > 0, \tag{3.11}$$

subject to

$$u_2(r_0) = u_0, \qquad u_2 \to 0 \qquad \text{as} \quad r \to \infty, \tag{3.12}$$

which gives

$$u_2(r) = u_0 \frac{K_0(r)}{K_0(r_0)} = u_2^{(1)}(r) \qquad \text{say.} \tag{3.13}$$

The functions $u_1^{(1)}$ and $u_2^{(1)}$ in (3.7) and (3.13) provide simple pointwise bounds for u and have been obtained by elementary means. The Debye–Hückel approximation mentioned in Section 1 corresponds to solving

(3.11) and (3.12), and so from this work we see that it actually provides an *upper* bound for u, this bound being $u_2^{(1)}$ in our notation. Our lower bound function $u_1^{(1)}$ in (3.7) appears to be new. Some values of these bounding curves for various values of the parameters r_0 and u_0 are given in Table I. We see that the bounds get farther apart as the value of u_0 is increased.

TABLE I

Bounding Functions $u_1^{(1)}$ and $u_2^{(1)}$

	$r_0 = 0.5, u_0 = 0.5$		$r_0 = 0.5, u_0 = 1.0$		$r_0 = 0.5, u_0 = 2.0$	
r	$u_1^{(1)}$	$u_2^{(1)}$	$u_1^{(1)}$	$u_2^{(1)}$	$u_1^{(1)}$	$u_2^{(1)}$
0.5	0.5	0.5	1.0	1.0	2.0	2.0
1.0	0.2252	0.2277	0.4355	0.4554	0.7586	0.9109
1.5	0.1131	0.1156	0.2118	0.2313	0.3225	0.4626
2.0	0.0596	0.0616	0.1081	0.1232	0.1440	0.2464
2.5	0.0323	0.0337	0.0567	0.0674	0.0662	0.1349
3.0	0.0178	0.0188	0.0303	0.0376	0.0310	0.0752
3.5	0.0099	0.0106	0.0164	0.0212	0.0147	0.0424
	$r_0 = 1.0, u_0 = 0.5$		$r_0 = 1.0, u_0 = 1.0$		$r_0 = 1.0, u_0 = 2.0$	
r	$u_1^{(1)}$	$u_2^{(1)}$	$u_1^{(1)}$	$u_2^{(1)}$	$u_1^{(1)}$	$u_2^{(1)}$
1.0	0.5	0.5	1.0	1.0	2.0	2.0
1.5	0.2512	0.2539	0.4863	0.5078	0.8501	1.0156
2.0	0.1324	0.1353	0.2482	0.2705	0.3797	0.5410
2.5	0.0717	0.0740	0.1302	0.1481	0.1745	0.2962
3.0	0.0395	0.0413	0.0695	0.0825	0.0816	0.1650
3.5	0.0221	0.0233	0.0376	0.0466	0.0387	0.0931
4.0	0.0124	0.0133	0.0205	0.0265	0.0185	0.0530
	$r_0 = 2.0, u_0 = 0.5$		$r_0 = 2.0, u_0 = 1.0$		$r_0 = 2.0, u_0 = 2.0$	
r	$u_1^{(1)}$	$u_2^{(1)}$	$u_1^{(1)}$	$u_2^{(1)}$	$u_1^{(1)}$	$u_2^{(1)}$
2.0	0.5	0.5	1.0	1.0	2.0	2.0
2.5	0.2708	0.2737	0.5246	0.5474	0.9189	1.0948
3.0	0.1493	0.1525	0.2802	0.3050	0.4300	0.6100
3.5	0.0834	0.0860	0.1515	0.1721	0.2038	0.3442
4.0	0.0470	0.0490	0.0827	0.0980	0.0975	0.1960
4.5	0.0267	0.0281	0.0455	0.0562	0.0470	0.1124
5.0	0.0152	0.0162	0.0251	0.0324	0.0228	0.0648

4. POINTWISE BOUNDS 2

Section 3 contains the best bounding curves based on a single chord and single tangent in the $u, f(u)$ plane. To improve on these it is necessary to introduce more elaborate functions f_1 and f_2. To illustrate this we choose continuous linear functions, with piecewise continuous derivatives, consisting of two chords and two tangents (see Fig. 2).

4.1. *Lower Bounding Function*

For the function f_1, which we shall denote by $f_1^{(2)}$, we take the chords joining the three points $(0, 0)$, $(v_1, f(v_1))$ and $(u_0, f(u_0))$ in the $u, f(u)$ plane, where v_1 is some number between 0 and u_0. Then

$$\begin{aligned} f_1^{(2)}(u) &= -\lambda_1^2 u, & 0 \leqslant u \leqslant v_1 \\ &= -\mu_1^2(u-u_0)+f(u_0), & v_1 \leqslant u \leqslant u_0 \end{aligned} \tag{4.1}$$

with

$$\lambda_1^2 = -\frac{f(v_1)}{v_1} = \frac{\sinh v_1}{v_1},$$

and

$$\mu_1^2 = -\frac{f(u_0)-f(v_1)}{u_0-v_1} = \frac{\sinh u_0 - \sinh v_1}{u_0 - v_1}. \tag{4.2}$$

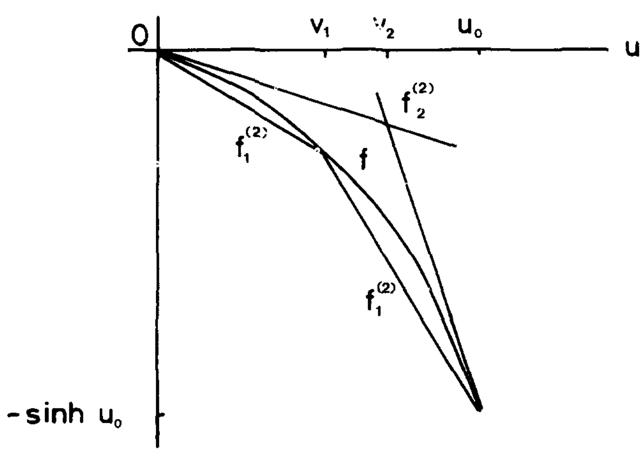

FIG. 2. Functions $f_1^{(2)}$ and $f_2^{(2)}$.

To find the corresponding lower bounding function u_1, we solve (2.9) with expression (4.1) for f_1, that is

$$\begin{aligned}\frac{1}{r}\frac{d}{dr}\left(r\frac{du_1}{dr}\right) &= \mu_1^2(u_1-u_0)-f(u_0), \qquad 0<r_0\leqslant r\leqslant r_1 \\ &= \lambda_1^2 u_1 \qquad\qquad\qquad\quad , \qquad r_1\leqslant r<\infty\end{aligned} \quad , \tag{4.3}$$

where r_1 is the value of r for which

$$u_1(r_1)=v_1, \tag{4.4}$$

and where

$$u_1(r_0)=u_0, \qquad u_1\to 0 \quad \text{as} \quad r\to\infty. \tag{4.5}$$

From (4.3) we find that

$$u_1(r)=u_1^{(2)}(r) \qquad \text{say,}$$

where

$$\begin{aligned}u_1^{(2)}(r) &= u_0+\frac{1}{\mu_1^2}f(u_0)+AI_0(\mu_1 r)+BK_0(\mu_1 r), \qquad 0<r_0\leqslant r\leqslant r_1, \\ &= CK_0(\lambda_1 r), \qquad r_1\leqslant r<\infty\end{aligned} \quad . \tag{4.6}$$

Here I_0 and K_0 are modified Bessel functions of the first and second kind [9], and we have imposed $u_1\to 0$ as $r\to\infty$. Making

$$u_1(r_0)=u_0 \tag{4.7}$$

and imposing the continuity conditions

$$u_1(r_1-)=u_1(r_1+)=v_1, \tag{4.8}$$

$$u_1'(r_1-)=u_1'(r_1+), \tag{4.9}$$

we obtain three equations for the three coefficients A, B and C with solution

$$A=A(\lambda_1,\mu_1,r_1)=\frac{1}{D}\begin{vmatrix} -\mu_1^{-2}f(u_0) & K_0(\mu_1 r_0) & 0 \\ -u_0-\mu_1^{-2}f(u_0) & K_0(\mu_1 r_1) & -K_0(\lambda_1 r_1) \\ 0 & \mu_1 K_1(\mu_1 r_1) & -\lambda_1 K_1(\lambda_1 r_1)\end{vmatrix}, \tag{4.10}$$

$$B = B(\lambda_1, \mu_1, r_1) = \frac{1}{D} \begin{vmatrix} I_0(\mu_1 r_0) & -\mu_1^{-2} f(u_0) & 0 \\ I_0(\mu_1 r_1) & -u_0 - \mu_1^{-2} f(u_0) & -K_0(\lambda_1 r_1) \\ \mu_1 I_1(\mu_1 r_1) & 0 & -\lambda_1 K_1(\lambda_1 r_1) \end{vmatrix}, \tag{4.11}$$

$$C = C(\lambda_1, \mu_1, r_1) = \frac{1}{D} \begin{vmatrix} I_0(\mu_1 r_0) & K_0(\mu_1 r_0) & -\mu_1^{-2} f(u_0) \\ I_0(\mu_1 r_1) & K_0(\mu_1 r_1) & -u_0 - \mu_1^{-2} f(u_0) \\ \mu_1 I_1(\mu_1 r_1) & \mu_1 K_1(\mu_1 r_1) & 0 \end{vmatrix}, \tag{4.12}$$

where

$$D = D(\lambda_1, \mu_1, r_1) = \begin{vmatrix} I_0(\mu_1 r_0) & K_0(\mu_1 r_0) & 0 \\ I_0(\mu_1 r_1) & K_0(\mu_1 r_1) & -K_0(\lambda_1 r_1) \\ \mu_1 I_1(\mu_1 r_1) & \mu_1 K_1(\mu_1 r_1) & -\lambda_1 K_1(\lambda_1 r_1) \end{vmatrix}. \tag{4.13}$$

By (4.4) and (4.6) the value of r_1 is determined by

$$C K_0(\lambda_1 r_1) = v_1 \tag{4.14}$$

in which C is given by (4.12) and v_1 is any number between 0 and u_0. For our calculations we shall take

$$v_1 = 0.5\, u_0. \tag{4.15}$$

Some values of the corresponding lower bounding function $u_1^{(2)}$ are given in Table II for various values of the parameters r_0 and u_0.

4.2. *Upper Bounding Function*

To obtain an improved pointwise upper bound u_2 for u we choose the function f_2, which we shall denote by $f_2^{(2)}$, to consist of parts of the tangents (see Fig. 2) to $f(u)$ at the points $(0, 0)$ and $(u_0, f(u_0))$. We suppose these tangents meet at

$$u = v_2. \tag{4.16}$$

Then

$$\begin{aligned} f_2^{(2)}(u) &= -\lambda_2^2 u \quad , && 0 \leqslant u \leqslant v_2 \\ &= -\mu_2^2 (u - u_0) + f(u_0), && v_2 \leqslant u \leqslant u_0 \end{aligned} \tag{4.17}$$

TABLE II

Bounding Functions $u_1^{(2)}$ and $u_2^{(2)}$

	$r_0 = 0.5, u_0 = 0.5$		$r = 0.5, u_0 = 1.0$		$r_0 = 0.5, u_0 = 2.0$	
r	$u_1^{(2)}$	$u_2^{(2)}$	$u_1^{(2)}$	$u_2^{(2)}$	$u_1^{(2)}$	$u_2^{(2)}$
0.5	0.5	0.5	1.0	1.0	2.0	2.0
1.0	0.2269	0.2276	0.4487	0.4548	0.8575	0.9059
1.5	0.1149	0.1156	0.2254	0.2309	0.4170	0.4601
2.0	0.0611	0.0616	0.1188	0.1230	0.2128	0.2451
2.5	0.0333	0.0337	0.0644	0.0673	0.1116	0.1342
3.0	0.0185	0.0188	0.0355	0.0375	0.0596	0.0748
3.5	0.0104	0.0106	0.0198	0.0212	0.0322	0.0422
	r_1	r_2	r_1	r_2	r_1	r_2
	0.9330	0.7411	0.9262	0.7328	0.9000	0.7046

	$r_0 = 1.0, u_0 = 0.5$		$r_0 = 1.0, u_0 = 1.0$		$r_0 = 1.0, u_0 = 2.0$	
r	$u_1^{(2)}$	$u_2^{(2)}$	$u_1^{(2)}$	$u_2^{(2)}$	$u_1^{(2)}$	$u_2^{(2)}$
1.0	0.5	0.5	1.0	1.0	2.0	2.0
1.5	0.2529	0.2538	0.4999	0.5067	0.9527	1.0078
2.0	0.1344	0.1352	0.2635	0.2699	0.4862	0.5369
2.5	0.0734	0.0740	0.1427	0.1478	0.2551	0.2939
3.0	0.0408	0.0412	0.0787	0.0823	0.1362	0.1638
3.5	0.0229	0.0233	0.0439	0.0465	0.0737	0.0924
4.0	0.0130	0.0133	0.0248	0.0265	0.0402	0.0526
	r_1	r_2	r_1	r_2	r_1	r_2
	1.5089	1.2900	1.4998	1.2800	1.4651	1.2457

	$r_0 = 2.0, u_0 = 0.5$		$r_0 = 2.0, u_0 = 1.0$		$r_0 = 2.0, u_0 = 2.0$	
r	$u_1^{(2)}$	$u_2^{(2)}$	$u_1^{(2)}$	$u_2^{(2)}$	$u_1^{(2)}$	$u_2^{(2)}$
2.0	0.5	0.5	1.0	1.0	2.0	2.0
2.5	0.2726	0.2735	0.5383	0.5459	1.0234	1.0842
3.0	0.1515	0.1524	0.2968	0.3042	0.5465	0.6041
3.5	0.0852	0.0860	0.1657	0.1716	0.2955	0.3408
4.0	0.0484	0.0490	0.0934	0.0977	0.1613	0.1941
4.5	0.0277	0.0281	0.0530	0.0560	0.0887	0.1113
5.0	0.0159	0.0162	0.0302	0.0323	0.0490	0.0642
	r_1	r_2	r_1	r_2	r_1	r_2
	2.5728	2.3305	2.5613	2.3189	2.5182	2.2792

with

$$\lambda_2^2 = -f'(0) = 1, \tag{4.18}$$

$$\mu_2^2 = -f'(u_0) = \cosh u_0. \tag{4.19}$$

Continuity of $f_2^{(2)}$ at $u = v_2$ requires that

$$-\lambda_2^2 v_2 = -\mu_2^2(v_2 - u_0) + f(u_0),$$

giving

$$v_2 = \frac{u_0 \cosh u_0 - \sinh u_0}{\cosh u_0 - 1}. \tag{4.20}$$

To find the corresponding upper bounding function u_2 we solve (2.10) with expression (4.17) for f_2, that is,

$$\left.\begin{aligned} \frac{1}{r}\frac{d}{dr}\left(r\frac{du_2}{dr}\right) &= \mu_2^2(u_2 - u_0) - f(u_0), \qquad 0 < r_0 \leqslant r \leqslant r_2 \\ &= u_2 \qquad\qquad\qquad\qquad\quad, \qquad r_2 \leqslant r < \infty \end{aligned}\right\}, \tag{4.21}$$

where r_2 is the value of r for which

$$u_2(r_2) = v_2, \tag{4.22}$$

and where

$$u_2(r_0) = u_0, \qquad u_2 \to 0 \quad \text{as} \quad r \to \infty. \tag{4.23}$$

Solving (4.21) and imposing the boundary conditions (4.23) and the continuity conditions

$$u_2(r_2-) = u_2(r_2+) = v_2, \tag{4.24}$$

$$u_2'(r_2-) = u_2'(r_2+), \tag{4.25}$$

we find that

$$u_2(r) = u_2^{(2)}(r) \qquad \text{say,}$$

where

$$\left.\begin{aligned} u_2^{(2)}(r) &= u_0 + \mu_2^{-2} f(u_0) + A_2 I_0(\mu_2 r) + B_2 K_0(\mu_2 r), \quad 0 < r_0 \leqslant r \leqslant r_2, \\ &= C_2 K_0(r), \qquad r_2 \leqslant r < \infty \end{aligned}\right\}. \tag{4.26}$$

Here the coefficients A_2, B_2, C_2 are given by

$$A_2 = A(\lambda_2, \mu_2, r_2), \qquad B_2 = B(\lambda_2, \mu_2, r_2), \qquad C_2 = C(\lambda_2, \mu_2, r_2), \quad (4.27)$$

these functions being defined in (4.10) to (4.12). By (4.22) and (4.26) the value of r_2 is determined by

$$C_2 K_0(r_2) = v_2 \qquad (4.28)$$

in which C_2 is given by (4.27) and v_2 by (4.20). Some values of the upper bounding function $u_2^{(2)}(r)$ in (4.26) for various values of the parameters r_0 and u_0 are given in Table II. As would be expected, the bounding functions $u_1^{(2)}$ and $u_2^{(2)}$ get farther apart as the value of u_0 is increased, but these bounds are much closer than those in Table I arising from the simple functions derived in Section 3.

It is clearly possible to obtain better agreement between the upper and lower bounding functions by increasing the number of line segments in the piecewise-linear functions approximating $f(u)$. However, we have shown that functions with only a pair of line segments can lead to quite good agreement and thus give a fairly accurate solution of a nonlinear boundary value problem.

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